



Final Report

COMPUTATION IN MECHANICS OF MATERIALS

(ONR Contract N00014-88-0676)

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The goal of this project, which was part of the DARPA Balanced Technology Initiative on Computational Mechanics, was to develop a comprehensive approach to the numerical modeling of the mechanical behavior of materials. Particular areas for focus in the project were the inelastic deformation of highly anisotropic materials such as single crystals and textured polycrystals, as well as evolving microstructural damage in ceramics and ductile metals in both slow and high rate deformation processes. While the contract was awarded for a period of four years, it was actually funded only for the first year plus a few months into the second year. Nonetheless, significant progress can be reported as a direct result of this project.

Nearly all of the funding for the project was used to upgrade an Alliant FX/8 minisupercomputer, purchased by Brown University in 1987, from a four processor unit with 24 megabytes of RAM to an eight processor unit with 56 megabytes of RAM plus suitable disc drives for data storage. This machine, which was an integral part of the Computational Mechanics Research Facility at Brown University, provided the opportunity for significant advance in computational research along the lines outlined in the original proposal. An annotated sampling of papers reporting research on computational mechanics of materials is provided below. Each of these papers included an explicit acknowledgment of the use of the Alliant computer in the work.

- Needleman, A., "Dynamic shear band development in plane strain", *Journal of Applied Mechanics*, vol. 111, 1989, pp. 1-9.

In this paper, plane strain compression of a rectangular block was used as a model problem to investigate the dynamics of shear band development from an internal inhomogeneity. The material was characterized as a von Mises elastic-viscoplastic solid, with a hardness function that exhibited a local maximum. Regardless of whether the material is hardening or softening, plastic strain development involved the evolution of fingerlike contours emanating from the inhomogeneity at 45 degrees to the compression axis. Once a given strain contour crossed the specimen, it fanned out about its initial direction of propagation. For a softening solid, this fanning out ceased for some strain level greater than the strain at the hardness maximum and further straining took place in an ever narrowing band. Many of the qualitative features of shear band development under dynamic loading conditions were found to be the same as under quasistatic loading conditions, but a significant retardation of shear band development due to inertial effects was found.

- Ortiz, M., Sotelino, E. D. and Nour-Omid, B., "Efficiency of group implicit concurrent algorithms for transient finite element analysis", *International Journal for Numerical Methods in Engineering*, vol. 28, 1989, pp. 2761-2776.

The performance of group implicit algorithms was assessed on the Alliant FX/8, taking full advantage of its concurrent computational mode. It was shown that, as

the number of subdomains was increased, performance enhancements were derived from two sources: the increased parallelism in the computation and a reduction in equation solving effort. Moreover, it was shown that these two performance enhancements are synergistic, in the sense that the corresponding speed-ups were multiplied, rather than merely added. The numerical simulations demonstrated that, if  $n$  is the number of degrees of freedom of the structure,  $p$  the number of processors used in the computations, and  $s \geq p$  is the number of subdomains in the partition, the net speed-up was found to be  $O(ps^{1/2})$  in two dimensions and  $O(ps)$  in three dimensions, asymptotically as  $n/s \rightarrow \infty$ . In particular, speed-ups with respect to Newmark's method of  $O(s^{1/2})$  in two dimensions and  $O(s)$  in three dimensions are obtained on a single-processor machine. Finally, simulations on a 32-node hypercube were also presented for which the interprocessor communication efficiencies obtained were consistently in excess of 90 percent.

- Ramesh, K. T. and Clifton, R. J., "Finite element analysis of pressure-shear plate impact experiments on elastohydrodynamic lubricants", *Journal of Applied Mechanics*, to appear.

Pressure-shear experiments on an elastodynamic lubricant (5P4E) were interpreted by means of a finite deformation theory of stress wave propagation in an elastic/viscoplastic material. Elastic response was modeled as that of a neo-Hookean solid, modified to include compressibility in such a way that the shock velocity increased linearly with increasing particle velocity. Viscoplastic response was modeled by means of an activation rate model in which the activation energy was taken to be pressure-sensitive. Parameters in the elastic model were determined from the rising part of the transmitted stress profiles, which are related to transit times for multiple reverberations through the thickness of the lubricant layer. Parameters in the viscoplasticity model were determined from the shear stress transmitted after nominally homogeneous states of stress were established throughout the thickness of the lubricant. Good agreement between measured and computed wave profiles was obtained over the entire range of pressures used in the experiments.

- Shih, C. F. and Asaro, R. J., "Elastic-plastic analysis of cracks on bimaterial interfaces: Part I - Small scale yielding", *Journal of Applied Mechanics*, vol. 55, pp. 299-316; "Part II - Structure of small-scale yielding fields", *ibid.*, vol. 56, pp. 763-779.
- Shih, C. F., Asaro, R. J. and O'Dowd, N. P., "Part III - Large scale yielding", *ibid.*, vol. 58, pp. 450-463.

In parts I and II, the structure of small-scale yielding fields of interface cracks were described in the context of small strain plasticity and  $J_2$  deformation theory of plasticity. These fields were found to be members of a family parameterized by the

plastic phase angle which also determined the shape or phase of the plastic zone. Through full-field analysis, the resemblance between the plane strain interface crack tip fields and mixed mode HRR fields in homogeneous materials was demonstrated. Part III was focused on states of deformation dominated by the tendency for the crack faces to open, and the scope of the study was broadened to include finite deformation plasticity and finite deformation effects on the near-tip fields. A geometrically rigorous formulation of  $J_2$  flow theory was adopted, taking full account of crack tip blunting. The results revealed several surprising effects that have important implications for fracture, associated with finite ligament plasticity and finite strains. For one thing the fields that developed near the bimaterial interfaces were more intense than those in homogeneous materials when compared at the same value of remote load. For example, the plastic zones, plastic strains, and the crack tip openings that evolved near bimaterial interfaces were considerably larger than those that developed in homogeneous materials. The stresses within the finite strain zone were also higher. In addition, a localized zone of high hydrostatic stresses developed near the crack tip but then expanded rapidly within the weaker material as the plasticity spread across the ligament. These stresses could be as much as 30 percent higher than those in homogeneous materials. Thus, the weaker material was subjected to large stresses as well as strains, states which promote ductile fracture processes. At the same time, the accompanying high interfacial stresses tended to promote interfacial fracture.

Other articles on related issues in computational mechanics of materials were also published, incorporating an acknowledgment to the Alliant computer, but the foregoing list is indicative of the kind of work that was accomplished during the period of funding.

In addition to its use for research purposes, the Alliant FX/8 was also used in a graduate course at Brown in order to introduce graduate students to parallel-vector computation strategies. This course, Engineering 234: *Computational Methods in Structural Mechanics*, was taught by Professor M. Ortiz and it impacted approximately 30 PhD students during the lifetime of the machine.

The Alliant FX/8 mini-supercomputer was taken out of service at Brown University in 1992. The architecture on which this machine was based was truly revolutionary when the machine became available, and it offered the most advantageous means for solving problems involving complex material behavior and geometrical effects. However, over the course of several years, this technology was overrun by RISC based workstation technology. The result was that the resale value of the Alliant computer fell rapidly over its five year lifetime, until it was virtually zero. Consequently, this machine was replaced by a local network of about 25 DEC workstations during a two year period and, once the computing power available in the Computational Mechanics Research Facility far exceeded that available with the Alliant, this machine was discarded. Thus, while it served a valuable and unique role in the evolution of the field of computational

mechanics of materials, the machine itself did not retain intrinsic value that could be recovered at the end of its useful lifetime.

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